ELECTROHYDRODYNAMIC MODEL OF ELECTRON MICROSCOPE

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Abstract: This work presents a complex multiphysics model of an electron microscope in ANSYS Fluent software. A custom electromagnetic model was used to describe the relativistic transport of electrons. The model consisted of a description of an electromagnetic field, relativistic transport of charged particles and interactions between charged particles and solid materials. Presented results suggest, that the custom model can be coupled with the CFD module, which results in a possibility of coupled simultaneous simulations of hydrodynamics, electromagnetics, and a transport of charged particles.

Keywords: Electron microscope, numerical modelling, ANSYS Fluent, relativistic transport

1 INTRODUCTION

An Electron microscope is a device used for studying a micro-structure, surface, and a chemical composition of specimens by an electron beam. Nowadays, the technology is well established in many industrial and scientific areas. Still, the design of an electron microscope is a very complex process, which combines many areas of physics. Experimental studies, which could help with designing and optimising electron microscopes, are often very difficult due to extreme operational conditions. On the other hand, numerical simulations are often able to study these processes, as they only require knowledge of the geometry and general operating and boundary conditions. Currently, the numerical simulations in electron microscopy are often focused only on one area of physics (electromagnetics, particle-matter interactions, or hydrodynamics) [1, 2, 3]. Usually, the individual investigation of one specific area will not bring any inconsistencies in the results, however in some cases the multiphysics nature of these processes might be very important. This is the case for environmental scanning electron microscopy (ESEM), which uses a higher pressure in the specimen chamber, which allows for the scanning of organic materials. For these microscopes, it is necessary to consider electron transport in the vacuum as well as its interactions with residual gas and the specimen. A huge amount of research is focused on the area of gas-particle interactions as it is a very complex phenomenon. However, the transport of electrons from the electron gun and the gas flow in the differentially pumped chamber is usually ignored [2, 3].

This paper presents a custom numerical model implemented into a CFD software ANSYS Fluent, which was shown to be able to successfully model the rarefied gas flow in an ESEM [3]. The custom model consists of a description of an electromagnetic field and a description of a relativistic electron transport. This model was used for simulation of a simplified electron microscope, which included generation of electrons, their focusing and their interaction with a specimen as well as the rarefied gas flow.

2 NUMERICAL MODEL

The presented numerical model consists of an in-built CFD module and a custom model describing electromagnetic field with relativistic electron transport. This model was used to study processes in a simplified electron microscope, which is described in Figure 1. The microscope consisted of a thermionic electron source, two focusing coils, differentially pumped chamber, scintillation detector and a specimen. The radius of the filament tip was 0.25 mm. The internal diameter of the coils was 26 mm, the external diameter was 78 mm, and the height was 65 mm. The diameter of all apertures was 0.5 mm. The distance between the filament tip and the specimen was 250 mm.

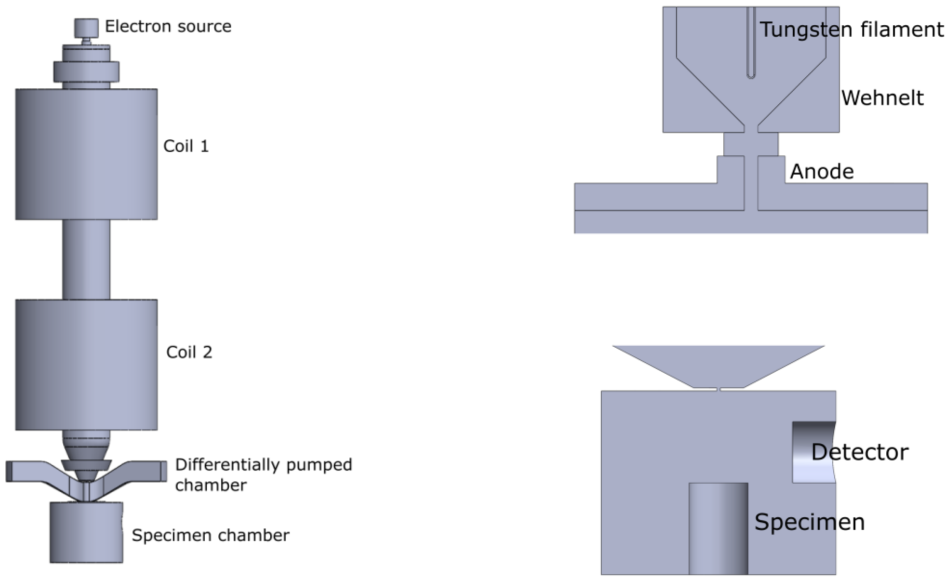

Figure 1: Simplified geometry of an electron microscope

2.1 GAS FLOW

Generally, any CFD software is based on the continuum assumption, which uses Navier-Stokes equations to describe a general fluid flow [4, 5]. As the pressure in the electron microscope is low, the gas might be so rarefied that the continuum assumption might not be applied. The Knudsen number, which describes the gas dynamics regime was calculated as in [6], in which the characteristic length was calculated locally as a ratio between density and the density gradient. The value of Knudsen number in this case was in range of 0 – 0.1 (maximum behind the apertures). These values represent continuum flow as well as the slip flow regime, which is still defined by Navier-Stokes equations. The adjustment considering the slip lies in the application of the Maxwell slip boundary for the velocity and the Smoluchowski temperature jump condition [7]. These boundary conditions were applied using a FLUENT's in-built option, which is available for laminar flows. In this case, the Reynolds number was sufficiently low, so the laminar flow assumption was valid. In the electron optics area, the vacuum is so high that the continuum assumption cannot be applied. To avoid this complication, the flow in this area was ignored and only constant pressure was considered. The gas density was described by the ideal gas law, while the viscosity was defined by the kinetic theory. The pressure boundary conditions were set as: 500 Pa in the specimen chamber, 30 Pa in the differentially pumped chamber and 0 Pa in the electron optics area. This simplification was used as this study describes only a general microscope and the exact vacuum pump parameters were not known.

2.2 ELECTROMAGNETIC FIELD

ANSYS Fluent offers a possibility of implementing custom user defined functions and user defined scalars (UDS), which are variables defined by a general transport equation. The electromagnetic field was described using an electric potential φ [V] and a magnetic vector potential $\boldsymbol{A}$ [V·s·m^{-1}]. These equations were implemented in a steady state manner using UDSs as [8]:

$$-\nabla^2\varphi = \frac{\rho_e}{\varepsilon} \quad (1)$$

$$-\nabla^2\boldsymbol{A} = \mu\boldsymbol{J} \quad (2)$$

Where is the charge density ρ_e [C·m^{-3}], ε is the permittivity [F·m^{-1}], μ is the permeability [H·m^{-1}] and $\boldsymbol{J}$ is the current density [A·m^{-2}].

The accelerating voltage was set to 10 kV (-10 kV at the tungsten filament and 0 V at the anode). The simplified scintillator was defined by a boundary condition of 300 V. The magnetic field of the coils was generated by total current density of $5\cdot10^7$ A·m^{-2} for the Coil 1 and $4.3\cdot10^7$ A·m^{-2} for the Coil 2.

2.3 ELECTRON TRANSPORT

Even though ANSYS Fluent includes a discrete phase model, which describes the transport of particles, it cannot be directly used for the simulation of the movement of charged particles as it always assumes that particles are in a flowing fluid. The original equation, which considered a constant mass of the particles and the drag force was adjusted to consider relativistic effect and the influence of the electromagnetic field [9]. The final equation of the relativistic electron transport was described as:

$$\frac{\partial \boldsymbol{v}}{\partial t} = \frac{q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})}{m_0\left(\frac{v^2}{c^2}{\gamma_L}^3 + \gamma_L\right)} \quad (3)$$

Where t is time [s], q is the charge [C], $\boldsymbol{E}$ is the electric field intensity [V·m^{-1}], $\boldsymbol{B}$ is the magnetic flux density [T], m_0 is the resting mass [kg], γ_L is the Lorentz factor [-].

The current density generated by the thermionic electron source was described by the Richardson-Dushmann equation, in which the material was defined as tungsten with a temperature of 2800 K [1]. Additionally, it was considered that primary electrons will release secondary electrons from the specimen. It was estimated that these secondary electrons had a random energy from 1 eV to 10 eV with a random direction pointing away from the specimen [10].

3 RESULTS

The simulation of particle trajectories in the studied electron microscope is shown in Figure 2. Without the focusing magnetic field, the particles naturally diverge, they do not reach the specimen chamber and are absorbed on the microscope walls. In the second case, electromagnetic coils are able to focus the electron beam on the specimen.

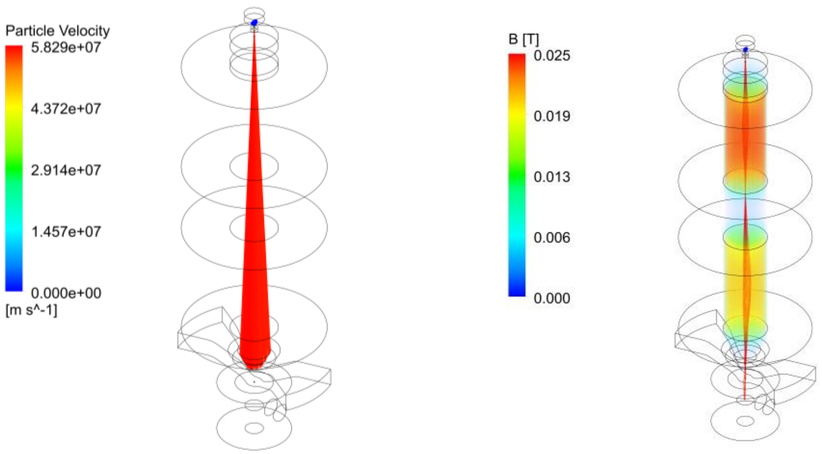

Figure 2: Electron trajectories without focusing coils (left) and with the magnetic field (right).

Figure 3 (left) shows the detail of electron source. It is possible to see the acceleration of electrons between the filament tip and the anode. As the particles are released from the filament, they are converging towards the crossover point and afterwards they start to diverge. Figure 3 (right) shows the detail of electron trajectories in the specimen chamber. While most of the primary electrons are scattered back at low angles, secondary electrons are released with random direction. Due to their low energy, these electrons are attracted by a simplified scintillation detector. Still, the low potential (300 V) at the detector cannot attract all secondary electrons.

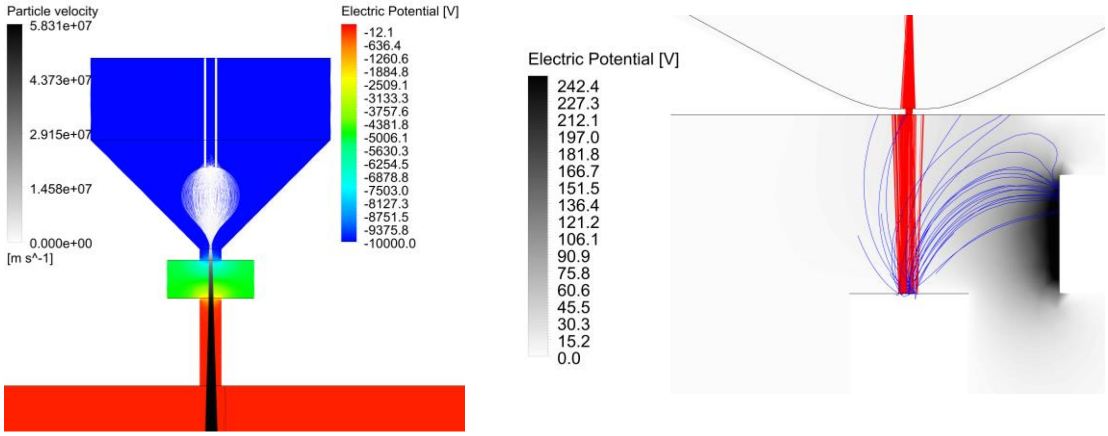

Figure 3: Detail of the electron source (left) and the detail of electron trajectories in the specimen chamber (right). In the specimen chamber, primary and back-scattered electrons are coloured red, while the secondary electrons are coloured blue.

Figure 4 show the gas velocity in the differentially pumped chamber. For better clarity, the displayed velocity is scaled to 100 m·s^{-1} (the maximum velocity was 460 m·s^{-1}). Due to the low pressure as well as the significant pressure difference between these chambers a supersonic choked flow can be observed [3]. As the gas moves through the aperture to the area with lower pressure, the velocity increases and the gas expands in all directions, which would not be visible for a subsonic flow in which only a narrow stream would be created. The supersonic flow forms at the end of the aperture and accelerates as it moves further away and is then decelerated to a subsonic flow by a shock wave.

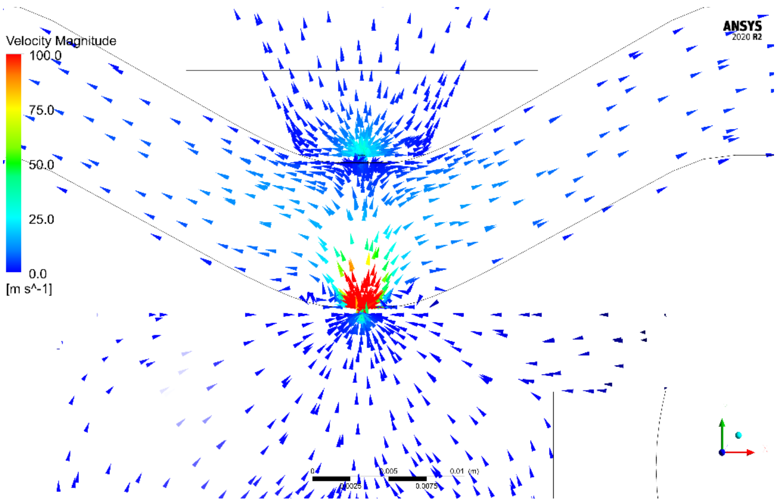

Figure 4: Rarefied gas flow in the differentially pumped chamber.

4 CONCLUSIONS

Numerical simulations of processes in electron microscopy can significantly help with designing and optimising new microscope parts as the experimental measurement might be often difficult or even impossible. The presented results show that the implemented custom model can describe the characteristic processes in an electron microscope. With this model, it might be possible to perform complex multiphysics simulations, which could increase the accuracy of the process description. From the gas flow simulation, it is possible to conclude that the flow regime significantly depends on the pressure and geometry conditions. While for some cases (high pressure), the continuum approximation with Navier-Stokes equations might be applicable, it is important to estimate the flow regime beforehand as there is a possibility that the Navier-Stokes equations will not be applicable. The presented electromagnetic model is able to describe the influence of electromagnetic field of trajectories of charged particles while considering relativistic effects. The theoretical velocity ($5.84\cdot10^{7}$ $m\cdot s^{-1}$) was in an agreement with velocity obtained from numerical simulations ($5.83\cdot10^{7}$ $m\cdot s^{-1}$). This model can be additionally extended with the description of stochastic particle-gas interactions to fully capture the whole process.

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